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A UNIFYING FRAMEWORK OF HOT SPOTS FOR ENERGETIC MATERIALS

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ABSTRACT

A one dimensional model of hot-spots is proposed to consider various regimes of ignition scenarios using a common platform. The model contains the most advanced features of spherical void collapse models. They include: viscoplastic heating, phase change, gas phase heating, finite-rate chemical reactions, and heat transfer between the locally heated zone and the surrounding mass. Test calculations, based so far on cyclonite (RDX) data, show that the model behavior is comparable to that of spherical void collapse model under shock loading condition. Results also show that chemical initiation under various mechanical excitation as well as thermal heating can be understood in a unified fashion; the initiation thresholds are summarized in terms of total energy deposited to the hot-spot, size of the hot-spot, and the rate of the energy deposition.

KEYWORDS

Explosive materials, Hot-spot ignition, Unifying framework

INTRODUCTION

The concept of "hot-spot" or the region of high energy localization was introduced by Bowden and Yoffe (1952) to explain the ignition of explosive materials when the mean field conditions are inadequate. For solid explosives, various mechanisms have been proposed for hot-spot formation, such as pore collapse, shear banding, friction, fracture, and jetting (Davis 1981; Dienes 1995; Kang et al., 1992; Massoni et al., 1999).

Currently much is unknown about how the formation of hot-spot is related to the initial material state and loading conditions. As a result, modeling of hot-spot formation involves a priori choice of a mechanism, which typically involves a model geometry that may not be representative of actual hot-spot geometry. But at present, there is no incontrovertible evidence to prefer

one mechanism over the others. In addition, single-mechanism approach can be problematic for complex systems like polymer-binder explosives (PBX).

Nevertheless, if one examines various models setting aside the mechanisms, a unifying framework can be identified. The framework consists of: (1) a region where mechanical energy is highly localized, (2) thermal mass surrounding the region described in (1), (3) creation or existence of the region occupied by gas, (4) heat flow between the regions, and (5) reaction chemistry in the gas, at the solid/gas interface, or both. In the present investigation, a hot-spot model was developed using the framework described above without being specific about the hot-spot formation mechanisms. Rather, attention is focused on whether the model yields results that are consistent with other mechanistic models by ranging over the parameter space, and how the model parameters affect the ignition conditions.

HOT-SPOT MODEL

Figure 1 shows an idealized model of hot-spot based on the unifying framework. The model is one dimensional and consists of three components: solid with a region of localized heating, gas cavity, and solid-gas interface. The solid is assumed to be incompressible. Thus, the solid moves with a common particle velocity, and the motion is determined by the balance of external loads, gas pressure, and configurational stress which represents the effect of contact force that may develop at the interface. The temperature is determined by the analytic solution of heat conduction equation for a fixed length domain. The heat is added uniformly to the zone of energy localization. It is noted that the width of the zone δ $(=b-a)$ and the rate of volumetric heating ϕ_s are free parameters, at present. In this way, the question of coupling between energy localization and the state of material is set aside for the moment.

The gas equations are obtained based on the assumption that average behavior is adequate for the present purpose. Reaction chemistry is assumed to be single step described by the Arrhenius kinetics model with pressure dependency. The equation of state is prescribed by a modified form of the ideal gas equation of state. Heat conduction between the gas phase and the interface is also considered.

At the interface, conservation conditions of mass, momentum, and energy are imposed. It is assumed that the interface is infinitely thin. Because of localized heating in the solid phase, a mass flux is produced at the interface as a function of the interface temperature. Part of the flux may go through instantaneous chemical reaction. Depending of the modeling needs, the localized heating can be generated at the interface with a known surface heating rate $\phi_{s,i}$.

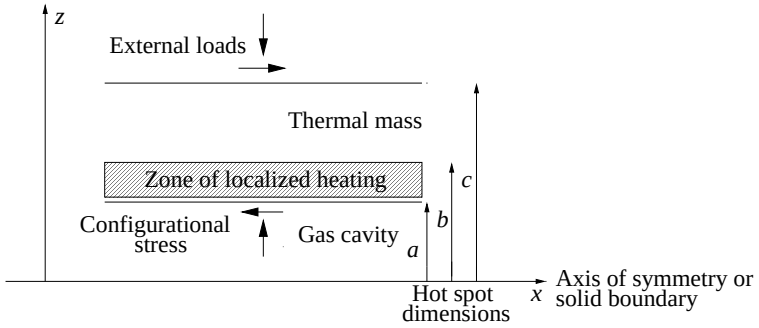

FIGURE 1. A schematic of the model structure. It consists of gas cavity, solid-gas interface, and solid with a zone of localized heating. Thick arrows represent stresses acting on the solid.

Mathematically, the model system consists of 7 ordinary differential equations and 10 algebraic equations. The differential equations were numerically integrated by Runge-Kutta scheme. The model contains all the features found in spherical pore collapse model by Kang et al. (1992). Major difference is that in their model, the energy localization is coupled with the model geometry whereas it is prescribed by free parameters in the present model. Details of the model are found in Yano et al. (2001).

MODEL SIMULATIONS

RDX was chosen for model simulations in order to compare the results with those of spherical void collapse calculation by Kang et al. (1992). Three sets of simulation results are presented in this section. The first two are results of ignition simulations with high and low heating rate. The last result presents a parametric study of critical ignition condition for RDX.

Figure 2 is a schematic of the conditions for ignition simulation where the rate of heating is high. The heating rate is indicative of the energy dissipation rate produced by spherical pore collapse under shock loading (Kang et al., 1992; Bonnet and Butler, 1996; Massoni et al. 1999). The magnitude of applied load and physical dimensions are from Kang et al. (1992). Figure 3 (a) and (b) show the results of the ignition simulation. At time $t = 0$, 1 GPa of external load is applied and the gas pore starts to collapse. At the same time, heat addition is started to the heating zone. The temperatures of the interface and the gas phase rise steadily. At 0.15 μs, the heat addition is terminated. The interface temperature starts to drop due to the termination,

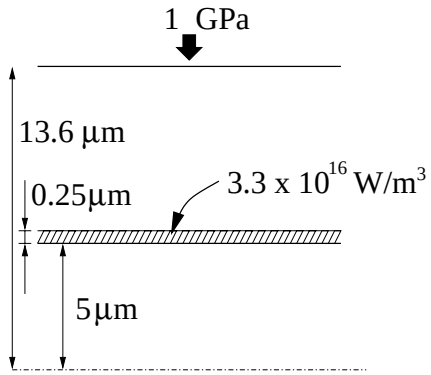

FIGURE 2. Conditions for ignition simulation with high rate of heating. The heating rate is indicative of energy dissipation rate of spherical pore collapse under shock loading condition.

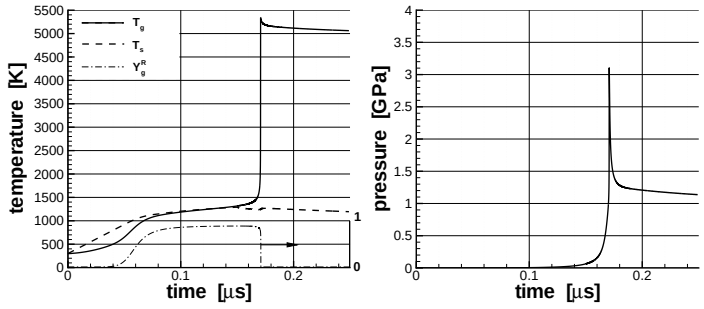

FIGURE 3. Results of ignition simulation for conditions shown in Fig. 2. (a) Time evolution of temperatures at the interface (thick dashed line) and in the gas phase (thick solid line). Thin dash-dotted line is the time evolution of reactant mass fraction in the gas phase. (b) Pressure evolution in the gas phase.

whereas the gas phase temperature keeps on rising because of exothermic chemical reaction in the gas phase. At about 0.17 μs, ignition takes place and both gas temperature and pressure rise in almost discontinuous manner. After the ignition, the gas pressure rapidly drops due to the expansion of the gas. Qualitatively and quantitatively, the ignition behaviors are very similar to those presented by Kang et al. (1992).

The conditions for the second simulation are shown in Fig. 4. In this simulation, the heat is added to the interface, and the heating rate is an estimate of frictional energy dissipation caused by low speed ($\sim$ 10 m/s) impact. Figure 5 (a) and (b) show the simulation results. The heat addition is maintained during $0 < t < 0.35$ ms for this calculation. Qualitatively, the results are similar to those of previous simulation, except the time scale for ignition is on the order of sub-millisecond. A plateau appeared in the pressure profile, because the gas pressure reached the external loading pressure, and the gas started to expand slowly. The plateau is not seen for higher external pressures.

Finally, the third results presents critical conditions for ignition. The idea of critical energy input is often pursued as a parameter to describe ignition conditions. One good example is the $p^2\tau$ criterion for explosives under impact loading where p is the shock pressure and τ is the time duration of the pressure (Walker,1985). Lee (1998), however, pointed out that the concept of critical energy alone is not sufficient to explain various ignition scenarios and that time factor over which the energy stimulus takes place must be considered. In this simulation, the critical energy deposited to the heating zone was calculated as a function of the size of heating zone and the rate of heating.

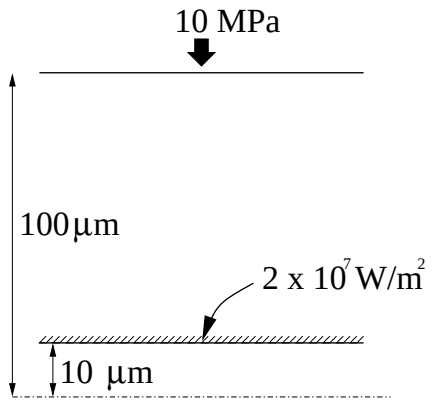

FIGURE 4. Conditions for ignition simulation with low rate of heating. The heating rate is comparable, in estimate, to frictional energy dissipation caused by low velocity impact.

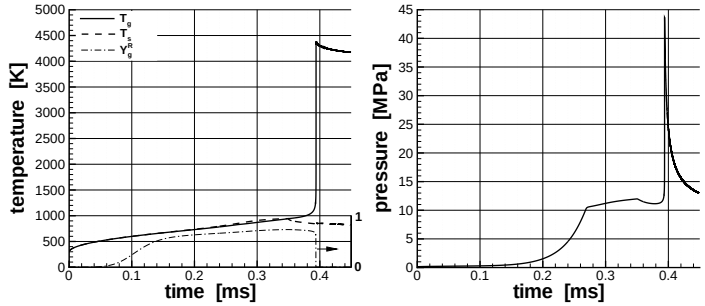

FIGURE 5. Results of ignition simulation for conditions shown in Fig. 4. (a) Time evolution of temperatures at the interface (thick dashed line) and in the gas phase (thick solid line). Thin dash-dotted line is the time evolution of reactant mass fraction in the gas phase. (b) Pressure evolution in the gas phase.

Figure 6 shows the results of parametric study. The symbols represent the points of critical conditions. For a given heating zone size and a heating rate, any energy above each symbol leads to ignition, and any energy below does not lead to ignition. The profiles are characterized by the existence of minima and convergence for large δ. In the left branch of the minimum point, less energy is required as δ gets larger. This is because heat loss at the interface due to conduction becomes smaller as the size of hot spot increases. On the other hand, in the right branch more energy is required for larger δ simply because of the volume increase. The curve approaches to linear profile for large values of δ as the effect of thermal conduction becomes negligible. The convergence behavior for large δ indicates that the ignition occurs once the interface temperature reaches the critical value (thermal ignition).

Three curves in Fig. 6 were obtained by curve fitting with the following fitting function.

$$E_{cr} = E_\infty + k_\infty[1 - \exp(-\alpha\phi_s\delta)]\delta + \frac{C_1}{(\phi_s\delta)^n}\exp(-C_2\phi_s\delta) \tag{1}$$

where E_{cr} is the critical energy and E_∞, k_∞, α, C_1, C_2, and n are fitting parameters. Values of the parameters used for the fitting are listed in Table 1.

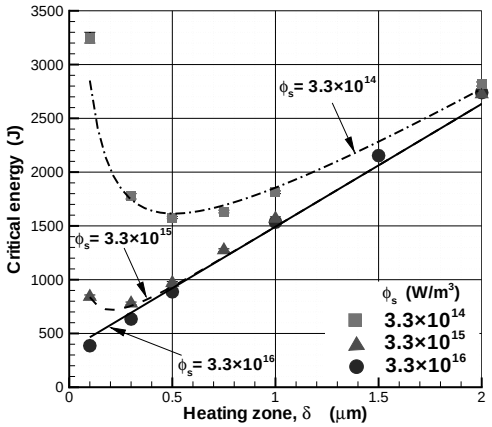

FIGURE 6. Critical condition for ignition in terms of total energy deposited to the heating zone as a function of the size of heating zone and heating rate. The symbols represent data obtained from parametric study, and the curves are the result of fitting using Eq.(1).

TABLE 1
VALUES OF PARAMETERS IN EQ.(1) USED FOR CURVE FITTING

variable (units)	value
E_∞ (J)	350
k_∞ (J/m)	1.142×10^{9}
α (1/W)	1.407×10^{-8}
n (—)	0.6
C_1 (J·W^n)	8.434×10^{7}
C_2 (1/W)	1.686×10^{-9}

CONCLUSIONS

An idealized model based on the unified framework described here produced ignition behaviors that are in general agreement with those of mechanism-specific models (Kang et al. 1992; Massoni et al. 1999). This agreement is seen over wide range of the parameter space, showing a consistent variation of time to ignition over orders of magnitude, depending on energy deposition rate and its duration. Further, a parametric study of critical ignition conditions shows results consistent to the observation by Field et al. (1992) on effective hot-spot ignition (hot-spot size: $0.1 - 10$ μm and duration of heating: $10^{-5} - 10^{-3}$ s). The results also show that critical ignition conditions are summarized in terms of total energy deposited to the hot-spot, the size of the hot-spot, and the rate of energy deposition.

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